United States Environmental Protection Agency **Office of Research and Development**

National Exposure Research Laboratory
FY02 Research Abstract

Government Performance Results Act (GPRA) Goal 1
APM 59

Significant Research Findings:

Addition of Toxic Polychlorinated Dibenzodioxins and Dibenzofurans to the Community Multiscale Air Quality (CMAQ) Model

Scientific Problem and Policy Issues	This research helps assess exposure to atmospheric emissions of Poly-Chlorinated Dibenzo-p-Dioxins and Dibenzo-Furans (commonly referred to as Dioxins and Furans, respectively). These pollutants are recognized sources of cancer. The atmosphere serves as a major pathway for human exposure because other exposures are believed to be slow and inefficient. Processes such as advection, diffusion, chemical transformation, gas to particle exchange, and wet and dry deposition have been incorporated into the Community Multiscale Air Quality (CMAQ) model. The model simulates the impacts of multiple emission sources on ambient air quality on spatial scales ranging from local to continental.
Research Approach	Researchers at the U.S. Environmental Protection Agency's National Exposure Research Laboratory have developed a new version of CMAQ to handle the treatment of seventeen Poly-Chlorinated Dibenzo-Furans and Dibenzo-p-Dioxins (PCDF's and PCDD's), expanding upon our previous research on atrazine with appropriate modifications to the treatment of dry deposition and atmospheric chemistry. Our implementation represents each congener's mass as divided between gaseous and aerosol species that exchange mass based on theoretical coefficients for gas to particle partitioning. The gaseous species undergo degradation based on congener-dependent rate constants and concentrations of hydroxyl radical (OH) as determined by the chemical mechanism employed in the CMAQ. The model is capable of simulating air concentration and deposition of PCDD's and PCDF's. While dry deposition removes all species, wet scavenging removes only particulate species. Our implementation makes the latter constraint because PCDD's and PCDF's have extremely low solubility in water. Deposition velocities for gas species have not been modified to include effects from organic factors since the time scales involved are still unknown.

Results and Implications

CMAQ was demonstrated with a simulation covering the early portion of July 1999. Model evaluation was conducted by comparing the percentage contribution from each congener to toxicity predicted by CMAQ with that reported in literature. Also, the predicted and reported coefficients for gas to particle partitioning have been compared. Absolute concentration levels simulated by CMAQ have also been compared with the observations from a national monitoring network. The results suggest that CMAQ is able to simulate the transport and fate of dioxins reasonably well. The model will be used for exposure assessments as part of the National Air Toxics Assessment (NATA) program.

Research Collaboration and Publications

Division staff conducted model development and testing in collaboration with scientists in the field. For example, Mark Cohen, of the National Oceanic and Atmospheric Administration's Air Resources Laboratory, provided data describing emissions of PCDD's and PCDF's and David Cleverly, of EPA's National Center for Environmental Assessment, provided monitoring data to support CMAQ evaluations. The information in the following papers was used as a template for handling the atmospheric transport and fate of PCDD's and PCDF's within CMAQ.

Cooter, E. J., and Hutzell W. T. (2002). "A Regional Atmospheric Fate and Transport Model for Atrazine, 1: Development and Implementation." *Environ. Sci. Technol.*; 36(19); 4091-4098.

Cooter, E. J.; Hutzell, W. T.; Foreman, W. T.; Majewski, M. S (2002). "A Regional Atmospheric Fate and Transport Model for Atrazine, 2: Evaluation." *Environ. Sci. Technol.;* 36 (21); 4593-4599.

Future Research

Additional simulations are needed to evaluate CMAQ's performance over longer time scales and for different seasons. An inter-agency project may support the goal through a model intercomparison project.

Contacts for Additional Information

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